

Quantum Entanglement Manifestation of Transition to Nonlinear Self-trapping for Bose-Einstein Condensates in a Symmetric Double-Well

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We investigate the nonlinear self-trapping phenomenon of the Bose-Einstein condensates (BEC) in a symmetric double-well, emphasizing on its behind dynamical phase transition. With increasing the nonlinear parameter depicting the interaction between the degenerate atoms the BEC turns to be self-trapped manifesting an asymmetric distribution of the atomic density profile. Essence of this phenomenon is revealed to be a continuous phase transition and underlying critical behavior is studied analytically and found to follow a logarithm scaling-law. We then go beyond the mean field treatment and extend to discuss the effect of the many-body quantum fluctuation on the transition. It is found that the transition point is shifted and the scaling-law is broken. In particular, the quantum phase transition is accompanied by the change of the entanglement entropy which is found to reach maximum at transition point. Behind physics is revealed.

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I. INTRODUCTION

Double-well system is a paradigm model used to demonstrate marvellous quantum tunnelling[1]. The realization of dilute Bose degenerate gas in last nineties provides a possibility of directly observing the tunnelling in the matter wave of macroscopic scale up to $100\mu m$ [2]. In Bose-Einstein condensates (BECs) system the interaction between the degenerate ultra-cold atoms plays an crucial role. It dramatically affects the quantum dynamics and leads to many unusual phenomena like nonlinear Josephson oscillation, nonlinear quantum tunnelling and critical onset in coherent oscillations, etc.[3, 4, 5, 6]. These problems have attracted much theoretical attention over the past few years and the recent realization of the BECs in the optical trap of a double-well configuration has brought a new research surge[7, 8].

Among many findings, the transition to self-trapping is most interesting one [9, 10, 11, 12, 13]. It says, with increasing the atomic interaction (repulsive), the Josephson oscillation between two wells is blocked, the BECs atoms in a symmetric double-well potential shows highly asymmetric distribution as if most atoms are trapped in one well. This phenomenon was observed in lab recently[8].

In this paper we achieve insight into this somehow counterintuitive phenomenon with addressing its behind phase transition and the influence of many-body quantum fluctuation on the phase transition. Analytically we identify the self-trapping phenomenon as a continuous phase transition and critical behavior is found to be characterized by a logarithm scaling-law. We then extend to discuss many-body quantum fluctuation effect on self-trapping. We find that, the transition point is shifted and the scaling-law is broken down due to the quantum fluctuation. Further investigations show that quantum properties are quite different for different interaction regions, such as self-trapping region and others. These properties can be well illustrated by entanglement entropy quantitatively. With employing average entropy as the or-

der parameter, we can clearly demonstrate the quantum phase transition: The entanglement entropy reaches its maximum at quantum transition point.

Our paper is organized as follows. In Sec.II, the self-trapping is studied within mean-field framework both analytically and numerically, revealing the critical behavior at the transition point. In Sec.III, we discuss the many-body quantum fluctuation effect and reveal the quantum entanglement manifestation of transition to nonlinear self-trapping. Sec.IV is our discussion and conclusion.

II. TRANSITION TO SELF-TRAPPING AND SCALING LAW

For two weakly coupled BECs trapped in a symmetric double-well, the system can be described by the so-called two-mode Hamiltonian [3, 14]

$$\hat{H} = \frac{\gamma}{2} (\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b}) + \frac{c}{2N} (\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b})^2 - \frac{v}{2} (\hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a}), \quad (1)$$

where the Bose operators $\hat{a}^{(\dagger)}$ and $\hat{b}^{(\dagger)}$ correspond to annihilating (creating) operators for different well respectively, $\gamma = E_a^0 - E_b^0$ is the energy bias between the two wells and $E_i^0 = \int \left(\frac{\hbar^2}{2m} |\nabla \varphi_i|^2 + V(r) |\varphi_i|^2 \right) dr$, $c = c_i = \frac{4\pi\hbar a N}{m} \int |\varphi_i|^4 dr$ denotes the effective interaction of atoms, $v = \int \left(\frac{\hbar^2}{2m} \nabla \varphi_a \nabla \varphi_b + V(r) \varphi_a \varphi_b \right) dr$ is the effective Rabi frequency which describes the coupling between two wells, N is total atoms number which is conserved, a is the s-wave scattering length, and φ_i ($i = a, b$) are wave functions for each well respectively. In the present work we focus on the case which has been realized in lab recently. For this case, the potential is symmetric so that $\gamma = 0$, and the interaction is repulsive, i.e., $c > 0$.

If the particle number is larger enough, the system can be well described in the mean-field approximation. Under mean-field approximation, the dynamics of the system is described by a classical Hamiltonian $H =$

$\langle \Psi_{GP} | \hat{H} | \Psi_{GP} \rangle / N$ (up to a trivial constant) in which $|\Psi_{GP}\rangle = \frac{1}{\sqrt{N!}} (a\hat{a}^\dagger + b\hat{b}^\dagger)^N |0\rangle$ is collective state of N -particle system [3, 14]. $a = |a|e^{i\theta_a}$ and $b = |b|e^{i\theta_b}$ are two c -numbers which correspond to the probability amplitudes of atoms in two wells respectively. By introducing the population difference $s = |b|^2 - |a|^2$ and the relative phase $\theta = \theta_b - \theta_a$, the classical Hamiltonian can be reduced to

$$H = -\frac{c}{2}s^2 + v\sqrt{1-s^2}\cos\theta, \quad (2)$$

where s and θ are canonical conjugate coordinates. Their equations of motions are

$$\dot{s} = v\sqrt{1-s^2}\sin\theta, \quad \dot{\theta} = -cs - \frac{vs}{\sqrt{1-s^2}}\cos\theta. \quad (3)$$

Self-trapping motion refers to the trajectories whose average population difference is not zero $\langle s \rangle \neq 0$. In the experiment [8], all the atoms are placed initially in one well, i.e., $s(0) = 1$ or -1 . As observed, with small interaction, the Josephson oscillation will be observed, and with larger interaction, the self-trapping emerges. This phenomenon can be well understood by the above classical Hamiltonian systems (2). Fig.1 plots the evolution of population difference s and its average for different interactions calculated by (3) with initial condition $s(0) = 1$. For c/v is smaller than 2, the population difference is oscillating symmetrically between 1 and -1 and its average is zero. However, for c/v is larger than 2, the motion is limited in half plane and the amplitude decreases with the interaction increasing, hence, the average of population difference will be nonzero and increasing with interaction.

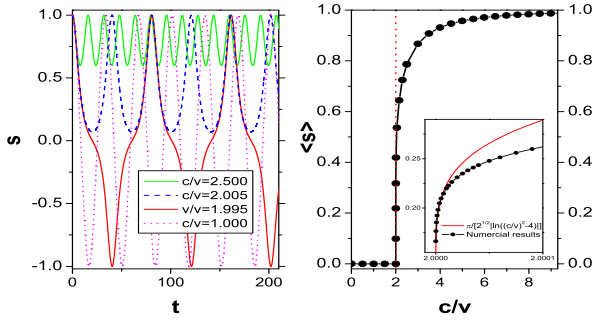


FIG. 1: (Color online) For initial condition $s = 1$, the population difference evolves with time for $c/v = 1, 1.995, 2.005, 2.5$ (left column), and the average of population difference vies parameter c/v (right column). Inset: the critical behavior near $c/v = 2$, the red line is for analytic formula (5) and the circles are for numerical simulation

The above process can be well understood from the analysis on the phase space of the classical Hamiltonian system. In Fig.2, we plot the trajectories in phase

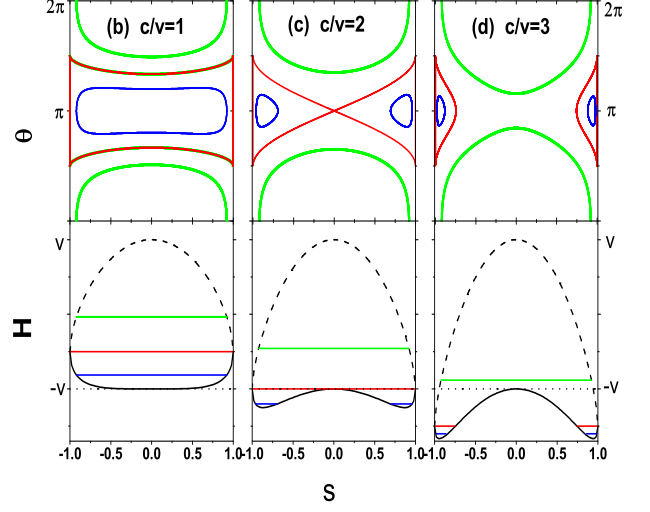


FIG. 2: (Color online) Trajectories on the phase space of the classical Hamiltonian system (2) (upper panels). In bottom panels we plot the energy profiles for the relative phase $\theta = 0$ (dashed) and $\theta = \pi$ (solid), respectively. The energies of the trajectories in upper panels are also denoted in bottom panels respectively using the lines with the same colors.

space and classical energy profiles for different parameters. The red lines correspond to the trajectories of which all the atom are initially in one well, i.e., $s(0) = 1$ or -1 . From this figure, we can see clearly that the dynamics transition happens at the moment when the energy of the trajectory with initial condition $s(0) = 1$ or -1 , $H(s = \pm 1) = c/2$, equals to the energy of the separatrix which is $H = -v$. When the energy of the trajectory initially in one well is larger than $-v$, one only finds Josephson oscillation trajectory, when for the energy being smaller than $-v$, the self-trapping happens.

For classical Hamiltonian system we can obtain the period T of a given trajectory by the integral $T = \oint \frac{\partial \theta}{\partial H} ds$, and average s of it by $\langle s \rangle = \frac{1}{T} \oint \frac{\partial \theta}{\partial H} s ds$, in which the integral path is along the trajectory. For the trajectory with initial condition $s(0) = \pm 1$, we have $H(s = \pm 1) = c/2$. Thus, from (2) and (3), we get

$$T = \begin{cases} 2 \int_{-1}^1 \frac{ds}{v\sqrt{(1-s^2)-[c(1-s^2)/2v]^2}} & c/v < 2 \\ 2 \int_{\sqrt{1-(2v/c)^2}}^1 \frac{ds}{v\sqrt{(1-s^2)-[c(1-s^2)/2v]^2}} & c/v > 2 \end{cases}, \quad (4)$$

and

$$\langle s \rangle = \begin{cases} \frac{2}{T} \int_{-1}^1 \frac{s ds}{v\sqrt{(1-s^2)-[c(1-s^2)/2v]^2}} & c/v < 2 \\ \frac{2}{T} \int_{\sqrt{1-(2v/c)^2}}^1 \frac{s ds}{v\sqrt{(1-s^2)-[c(1-s^2)/2v]^2}} & c/v > 2 \end{cases}, \quad (5)$$

in which we have used the formula $\cos\theta = c\sqrt{1-s^2}/2v$.

After some elaboration, we obtain

$$\langle s \rangle = \begin{cases} 0 & c/v < 2 \\ \frac{\pm \pi \sqrt{(c/v)^2 - 4}}{2c/v \operatorname{Im}\{K[(c/v)^2 / ((c/v)^2 - 4)]\}} & c/v > 2 \end{cases}, \quad (6)$$

where $K(x)$ is the complete first kind of elliptic integral. Near the transition point, it exhibits the logarithmic critical behavior

$$\langle s \rangle \approx \pm \frac{\sqrt{2}\pi}{c/v \ln[(c/v)^2 - 4]}. \quad (7)$$

The inset figure of Fig. 1 plots this critical behavior, where theoretical result is confirmed by numerical result obtained by numerically solving Eq.(3) with 4th-5th step-adaptive Runge-Kutta algorithm.

Our logarithmic critical behavior is very similar to the critical behavior in the measure synchronization in coupled Hamiltonian systems [15]. This is because critical behavior in both case is closely related to the separatrix of the Hamiltonian. Near the separatrix the period of the trajectory diverges to infinity, as the function of the relative deviation of the energy from the separatrix energy, its divergency follows a logarithm law[16].

In the above discussion, the initial state is set as $s = 1$, in fact for any initial state denoted by s_i, θ_i the transition to self-trapping occurs at some interaction parameter, and the critical behavior follows the same logarithm. If we extend the above discussion to this general case, we can obtain the general criterion for the occurrence of the self-trapping, i.e., $H(s_i, \theta_i, c, v) < -v$. Then, the critical point is expressed as,

$$\left(\frac{c}{v}\right)_{cr} = 2(1 + \sqrt{1 - s_i^2 \cos \theta_i}) / s_i^2. \quad (8)$$

From the above analytic expression, we see that, for the initial state with smaller population difference it requires stronger nonlinearity so that self-trapping occurs. Moreover, the critical point can be adjusted by the relative phase between the two weakly linked BEC in double-well. For example, for the case the population difference is 0.5, the critical point approximates to 15 and 8 for $\theta_i = 0$ and $\pi/2$, respectively. In practical experiments, the relative phase can be adjusted with using 'phase-imprinting' method, i.e., shedding un-uniform laser light on the BECs in double-well. This method has been successively applied to generate the dark solitons in cigar-shape BECs[17].

III. MANY BODY QUANTUM FLUCTUATION EFFECTS

In the mean field treatment we assume that the number of particle is large enough. However, in practical experiment, the particle number is finite, in order to know the quantum fluctuation effect due to finite particle number, we should investigate the self-trapping within the framework of the many body quantum system (1)[18, 19].

In treating the quantum many-body problem it is helpful to bear in mind some results from the quantum information theory concerning the entanglement [20]. The quantum entanglement is realized not only to be a crucial resource that allows for powerful communication and computational tasks that are not possible classically, but also to be a signal for quantum long-range correlation and therefore can serve as indicator for the quantum transition in concrete solid system[21]. Recent years witness growing interests in studying the interplay between entanglement and quantum phase transition[22, 23, 24, 25, 26].

Previously, some efforts have been devoted to study the dynamics of the BECs in double-well with full quantum treatment [27, 28]. In Ref.[27] the authors presented a quantum phase-space model of the BECs in a double-well potential by using the Husimi distribution function. They showed a good correspondence between the phase space of classical Hamiltonian (2) (mean-field approximation) and the quantum phase-space of two-mode hamiltonian (1) (full quantum framework). The authors of Ref. [28] calculated the time evolutions of states and their corresponding entanglement with different initial states for several different interactions between atoms. The time evolutions of entanglement entropy presented in Ref.[28] for several interactions between atoms show a decreasing tendency with increasing interactions.

In our following discussions of this section, however, we focus on the critical behavior at the transition to self-trapping as revealed by the above discussions, addressing how the quantum fluctuation influence on the transition behavior. As will be shown latter, the transition point is shifted and the scaling-law is broken down due to the quantum fluctuation. With increasing the atom number, the transition behavior demonstrates a perfect classical quantum correspondence. We also calculating the entanglement entropy achieving insight into the quantum transition. Our calculations on the time evolutions of entanglement entropy confirm the results of [28], and our further calculations on the time averaged entanglement strongly suggest that the entanglement entropy of this system serve as a good order parameter to describe such quantum transition.

A. Quantum Phase Transition

In the quantum framework the evolution of the system is governed by the Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \quad (9)$$

where $|\psi(t)\rangle = \sum_{n=0}^N a_n |n, N-n\rangle$, $|n, N-n\rangle = \frac{1}{\sqrt{n!(N-n)!}} (\hat{a}^\dagger)^n (\hat{b}^\dagger)^{N-n} |0\rangle$ ($n = 0, \dots, N$) are Fock states, and a_n are the probability amplitudes respec-

tively. Hence, the population difference is given by

$$s = \sum \frac{|a_n|^2 (N - 2n)}{N}. \quad (10)$$

We choose $|0, N\rangle$ as the initial state in the full quantum framework, which corresponds to $s = 1$ in the mean field model. In Fig. 3, we plot the average population difference calculated from the above Schrödinger equation for different total particle numbers. From the above calculation, we find that, the quantum fluctuation has two significant effects on the transition to self-trapping. First, the critical point is shifted to the left-hand side due to the finiteness of the particle number. From Fig.3, it is clearly seen that, keeping parameters c, v as constant, with increasing the number of the atoms, the transition point clearly shift to left-hand. For example, for $N = 50$, the transition point shifts to $c/v = 1.6$. We know that the quantum fluctuation closely relates to effective planck constant, here for this model it is $\frac{2}{N}$ [29]. Therefore we expect the deviation from the mean field critical point should be inversely proportional to total atom number. This prediction is confirmed by our calculations as shown in the inset of Fig.3. in which δ is the difference between the quantum transition point and the mean field one.

Secondly, the logarithm scaling-law is broken down by the quantum fluctuation. In Fig.3 we find the quantum fluctuation destroys the logarithm scaling-law of the mean field and no clear scaling-law is observed for the quantum case. With increasing the atom number the quantum results tends to the mean field results in the limit $N \rightarrow \infty$, as required by the classical quantum correspondence principle[29].

We should address that in the above calculation time period for average should be much longer than the period of the fastest oscillations but shorter than the period of the shortest quantum beating. This is because, essentially, the dynamics of quantum system is periodic or quasi-periodic, therefore, any dynamical effects of quantum system depends on the time scales [18, 30]. In our problem, there are two time scale, one is for integrating classical equation (3), the other is for integrating quantum equation (10), the later is N times the former one. In our calculations, the average time is $50N$, meaning that the corresponding classical time scale is same ($=50$). On the other hand, we find that, the averaged population difference increases gradually to 0.001 and then soars up. This is different from the mean field situation, where the averaged population difference keeps zero and then turns to be nonzero after critical point. So, in the quantum case, we define the transition point as the point that the averaged population difference is larger than 0.001. This observation also suggests that the no scaling-law for the finite particle situation.

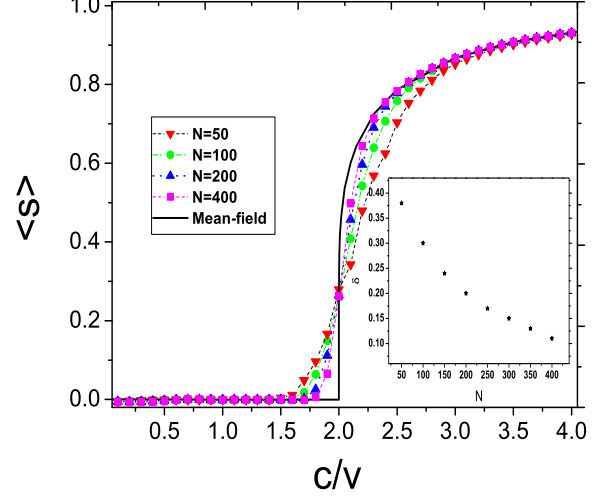


FIG. 3: (Color online) The average of population difference vies the parameter c/v obtained by full quantum simulations. Here, the initial state is $(n = 0, \dots, N)$, namely $s = 1$. Inset: the shift of the critical point comparing with meanfield predication δ for different atom number.

B. Entanglement Manifestation of the Quantum Phase Transition

To well understand the self-trapping phenomenon in full quantum description, we calculate evolution of the occupations on Fock states $|n, N - n\rangle$ ($n = 0, \dots, N$). Fig. 4 shows the evolution of Fock state occupation for different interactions. The horizontal axis is the time t , the vertical axis is the index of Fock state, namely, n corresponds to $|n, N - n\rangle$, and the contour is for the occupation probability. Fig. 4(a) is for the linear case, which shows the occupations are oscillating between $|0, N\rangle$ to $|N, 0\rangle$. For $c = 1.95$ (seeing Fig.4(b), near the transition point, we see that the wavefunction spread much rapidly to all the Fock states. Fig. 4(c) is plotted for the self-trapping case, $c = 2.5$, from which we see that the occupations is narrowed in partial Fock states, so that the average of population difference is nonzero.

From Fig. 4, we also see that the dynamics properties of such a quantum system are quite different for different interaction regions. To achieve more insight into the quantum transition to the self-trapping, we introduce the quantum entanglement entropy. For the system with the wave function $|\psi\rangle = \sum_{n=0}^N a_n |n, N - n\rangle$, its density operator is given by

$$\rho = |\psi\rangle \langle \psi| = \sum_{n,m} a_n a_m^* |n, N - n\rangle \langle N - m, m|, \quad (11)$$

Taking the partial trace with respect to one well yields

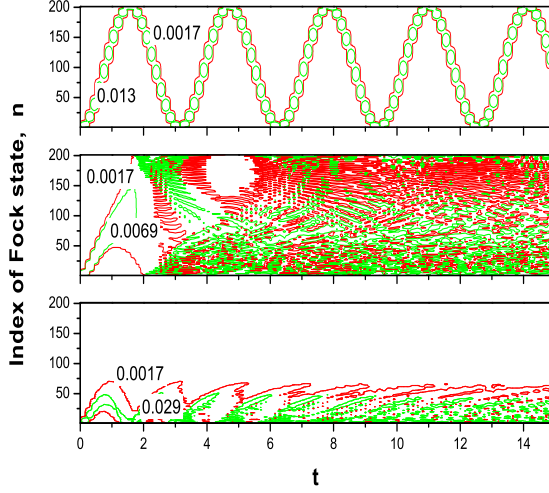


FIG. 4: (Color online) Occupations on Fock states for different time. The contours denote the probabilities of occupations. From up to bottom, $c/v = 0, 1.995, 2.5$ respectively.

the reduced density operator for the other,

$$\rho_a = \sum_n |a_n|^2 |n\rangle \langle n|. \quad (12)$$

Thus, the entropy of entanglement between the two coupled BEC's is given by [19]

$$E(\rho) = - \sum_{n=0}^N |a_n|^2 \log |a_n|^2. \quad (13)$$

The entanglement entropy has the following properties: it reaches maximum $E(\rho) = \log N$ when $|a_n|^2 = \frac{1}{N}$, and its minimum $E(\rho) = 0$ when $|a_n|^2 = 1$ and others are zero.

Because the self-trapping is dynamic phenomenon, the occupation on each Fock state is varied in time, therefore, we use average entropy. Technically, we have two choices to average it: we can average occupation firstly and then calculate entropy, and calculate entropy firstly then average it. So, we denote

$$E_{av} = - \sum_{n=0}^N \langle |a_n|^2 \rangle \log \langle |a_n|^2 \rangle / \log N, \quad (14)$$

and

$$\langle E \rangle = \left\langle - \sum_{n=0}^N |a_n|^2 \log |a_n|^2 \right\rangle / \log N. \quad (15)$$

The above formula have been normalized by $\log N$.

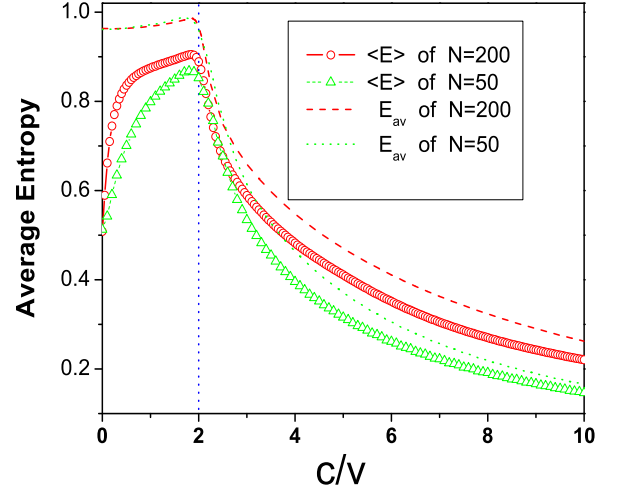


FIG. 5: (Color online) The entanglement entropy for different c/v . The circle line is for E_{av} and dashed line for $\langle E \rangle$

In Fig. 5, we plot the two kinds of average entropy with different interaction. Obviously, the dynamics of the quantum system can be well illustrated by the average entropies in quantities. For the linear case, the atoms mainly occupy several Fock states at a given time (see Fig. 4 (a)), and the occupied states are changed with time. Thus, the instantaneous entropy is small, so does the average entropy $\langle E \rangle$. On the other hand, because the average population on each Fock state are almost equivalent for this case, so E_{av} should be large. With the interaction increasing, the occupations on Fock states extend so that the instantaneous entropy increases. However, when the interaction exceeds the transition point self-trapping occurs and the occupations are limited on several Fock states (see Fig.4 (c)), hence, the instantaneous entropy becomes small, so does $\langle E \rangle$. For the same reason E_{av} will be small for self-trapping cases. From Fig. 5, we also observe that E_{av} is almost independence of the particle number and varies very little with changing the interaction parameter before it reaches its maximum. After that, it shows quite sensitive on the particle number as well as the interaction parameter. Whereas, for the entropy $\langle E \rangle$ before and after the maximum point it shows strong dependence of the particle number.

It is interesting that the two average entropies reach their maximum at the point very close to the transition point of mean field $c/v = 2$. This is very similar to phase transition of spin systems, where the phase transition happens at the point when entanglement of system reaches maximum [24]. This is different to the situation of the two-impurity Kondo model where the entanglement vanishes at a quantum critical point[25]. In particular, we find that, the maximum points of the aver-

age entropies varies very little with changing the particle number. The property suggests that the entanglement entropy is a better quantity than the average population in serving as an indicator to quantum phase transition, because the latter is too sensitive on the particle number as shown in Fig.3.

IV. DISCUSSION AND CONCLUSION

In conclusion, we have made thoroughly analysis on the transition to self-trapping for BECs confined in a symmetric double-well. Analytically we identify it as a continuous phase transition, where the time averaged population difference between two wells changes from zero to nonzero following a logarithm law at a critical point. We also discuss influence of the many-body quantum fluctuation on the transition to self-trapping. We find that the transition point is significantly shifted by quantum

fluctuation and no scaling-law is observed in quantum description. We investigate the quantum entanglement manifestation of the transition and find that the entanglement entropy reaches its maximum at the transition point. Classical quantum correspondence in the transition process is discussed.

V. ACKNOWLEDGMENTS

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